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Technical note: Revisiting the geometric theorems for volume averaging

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ABSTRACT

The geometric theorems reported by Quintard and Whitaker [5, Appendix B] are re-examined. We show (1) The geometrical theorems can be interpreted in terms of the raw spatial moments of the pore structure within the averaging volume. (2) For the case where the first spatial moment is aligned with the center of mass of the averaging volume, the geometric theorems can be expressed in terms of the central moments of the porous medium. (3) When the spatial moments of the pore structure are spatially stationary, the geometrical theorems allow substantial simplification of nonlocal terms arising in the averaged equations. (4) In the context of volume averaging, the geometric theorems of Quintard and Whitaker [5, Appendix B] are better interpreted as statements regarding the *spatial stationarity* of specific volume averaged quantities rather than an explicit statement about the media *disorder*.

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1. Introduction

In an early paper, Richard Feynman wrote about his interest in using multiple approaches to explain physics by stating [1].

> It is felt, in the face of daily experimental surprises for meson theory, that it might be worth while to spend one's time expressing electrodynamics in every physical and mathematical way possible...This is one reason that this paper is published, even though it is little more than a mathematical re-expression of old material. A second reason is the desire to describe a mathematical method which may be useful in other fields.

As Feynman recognized, the re-investigation of results by using multiple methods has tremendous pedagogical value. Throughout his career as a scientist, Steve Whitaker has applied similar ideas in his work in attempting to communicate ideas to experts and to students who were new to the material being discussed. Steve has a penchant for explaining things in ways that have enormous intuitive value, and he has never shied away from using these approaches to reach students and others just learning new material. At the same time, Steve has always been a proponent for rigor. Many of us who are familiar with Steve have heard him utter "If it is true, then there is a proof ..."

As an example of this multi-pronged approach, one can examine the multiple methods by which he has investigated proofs for the averaging theorem. Steve presented his version of the theorem first in 1967 [2], a more technically mature version in the context of real analysis [3], a version based on geometric principles appropriate for students [4], and a version proved using the theory of distributions [5].

This technical note is offered in much the same spirit. In this note, the geometrical theorems presented by Quintard and Whitaker [5, Appendix B] are examined in additional detail. The primary purpose of this note is to bring some additional perspective to the geometric theorems in a manner that is consistent with Steve's own penchant for re-visiting results. In particular, in this work we show (1) The geometrical theorems can be interpreted in terms of the raw spatial moments of the pore structure within the averaging volume; (2) For the case where the first spatial moment is aligned with the center of mass of the averaging volume, the geometric theorems can be expressed in terms of the central moments of the porous medium; (3) When the spatial moments of the pore structure are spatially stationary, the geometrical theorems allow substantial simplification of nonlocal terms arising in the averaged equations; and (4) In the context of volume averaging, the geometric theorems of Quintard and Whitaker [5, Appendix B] are better interpreted as statements regarding the *spatial stationarity* of specific volume averaged quantities rather than an explicit statement about the media *disorder*.

The geometric theorems presented by Quintard and Whitaker [5, Appendix B] are useful in making various simplifications for upscaling transport equations in multiphase media using the method of volume averaging (MVA) [6]. As originally presented, the proof of the associated theorems was elegant, but was not the kind of constructive proof that often appeals to students and to those interested in applications. In this short note, we also provide some direct examples indicating how one might constructively verify the proofs. As a second purpose for this note, some technical details about the functional dependence of the geometric

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Nomenclature

$\mathscr{A}_{\gamma\kappa}(\mathbf{x})$	domain of the fluid–solid interface within the averaging region $\mathscr{V}(\mathbf{x})$
$c_{A\gamma}(\mathbf{r},t)$	microscale concentration field of chemical species A in the γ-phase, mol/m^3
$\langle c_{A\gamma}\rangle^{\gamma}\|_{(\mathbf{x},t)}$	intrinsic averaged concentration field of chemical species A, mol/m^3
$\tilde{c}_{A\gamma}(\mathbf{r},t)$	$= c_{A\gamma}(\mathbf{r},t) - \langle c_{A\gamma}\rangle^{\gamma}\|_{(\mathbf{r},t)}$ concentration deviation field of chemical species A, mol/m^3
$\mathscr{D}_{\gamma}$	molecular diffusion coefficient, m^2/s
f	generic spatial scalar field
$\mathscr{G}(\mathbf{r},t)$	boundary condition source term, mol/m^2·s
$\mathscr{I}(\mathbf{r})$	initial distribution of $c_{A\gamma}$ within a catalyst pellet, mol/m^3
$\mathbf{I}$	the identity tensor
ℓ_{γ}	the characteristic length of the catalyst pore, m
ℓ	size of the side of a square periodic unit cell, m
L	characteristic length associated with a catalyst pellet (macroscale), m
$L_{\mathbb{C}}$	characteristic length associated with a catalyst pellet (macroscale), m
L_{m_n}	characteristic length associated with a catalyst pellet (macroscale), m
$m_n(\mathbf{x})$	the scalar magnitude field of M_n, m
$M_n(\mathbf{x})$	nth moment field of the pore space (or, alternatively, the indicator function Φ_{γ}); a tensor of order n, m^n
$\mathbf{n}_{\gamma\kappa}(\mathbf{r})$	unit normal vector directed from the γ-phase toward the κ-phase
O	fixed point of reference on an averaging volume used to locate it independently of the centroid
$\mathbf{O}$	order of magnitude symbol
$\mathbf{r}$	position vector, m
r_0	radius of the averaging region, m
t	time, s
$\mathscr{V}_o$	domain of an averaging volume using a reference point fixed to a unique reference point in the domain
$\mathscr{V}_{\gamma}(\mathbf{x})$	domain of the fluid phase within the averaging volume, $\mathscr{V}(\mathbf{x})$
$\mathscr{V}(\mathbf{x})$	$= \mathscr{V}_{\gamma}(\mathbf{x}) \cup \mathscr{A}_{\gamma\kappa}(\mathbf{x}) \cup \mathscr{V}_{\kappa}(\mathbf{x})$, domain of an averaging volume
$\mathscr{V}_{\gamma}(\mathbf{x})$	domain occupied by the γ-phase within the averaging volume $\mathscr{V}(\mathbf{x})$
V	volume of the averaging domain $\mathscr{V}(\mathbf{x})$, m^3
$V_{\gamma}(\mathbf{x})$	volume of the γ-phase contained within the averaging domain $\mathscr{V}(\mathbf{x})$, m^3
$\mathbf{w}$	position vector locating the unique point O to identifying the domain $\mathscr{V}$, m
$\mathbf{x}$	position vector locating the center of mass of the domain $\mathscr{V}$, m
$\mathbf{y}(\mathbf{r};\mathbf{x})$	position vector indicating the distance from $\mathbf{r}$ to $\mathbf{x}$; the explicit dependence upon $\mathbf{x}$ is sometimes suppressed for notational convenience
$\langle\mathbf{y}\rangle\|_{\mathbf{x}}$	first moment of the pore space computed with respect to the centroid of the averaging volume, $\mathscr{V}, m$

Greek symbols

$\varepsilon_{\gamma}(\mathbf{x})$	volume fraction (porosity) field of the fluid phase
$\boldsymbol{\lambda}$	unit directional vector
$\Gamma_n(\mathbf{x})$	repeated outer vector product field defined by Eqs. (18) and (19)
$\Phi_{\gamma}(\mathbf{x})$	γ-phase indicator function
$\boldsymbol{\Pi}$	repeated outer product symbol defined by Eq. (79)
$\rho_{\mathbb{C}}(\mathbf{x},t)$	autocorrelation function for the concentration field $c_{A\gamma}$
$\rho_{m_n}(\mathbf{x})$	autocorrelation function for the scalar magnitude field m_n
$\mu_n(\mathbf{x})$	the n^{th} central moment of the pore space (or, alternatively, the indicator function Φ_{γ}); a tensor of order n, m^n
(ζ,η,ξ)	components of a position vector, m

Symbols

∇	gradient operator with respect to the variable $\mathbf{x}$
∇_r	gradient operator with respect to the variable $\mathbf{r}$
$\otimes$	the outer product symbol; $\mathbf{a}\otimes\mathbf{b} = a_i b_j$

Subscripts

A	an index, unique for each chemical species
γ	associated with the fluid phase
κ	associated with the fluid phase
$\gamma\kappa$	associated with the solid–fluid interface
ζ	ζ-component of a vector quantity
η	η-component of a vector quantity
ξ	ξ-component of a vector quantity
Note:	Generally microscale quantities are generally referenced to the spatial coordinate $\mathbf{r}$; macroscale quantities are generally referenced to the spatial coordinate $\mathbf{x}$.

quantities involved in the method of volume averaging are given additional clarification.

2. Geometric theorems: an example via upscaling diffusion

The process of diffusion (and diffusion-like processes) is one of the archetypical problems for upscaling in porous media. This problem has been studied for literally hundreds of years (see the excellent review of this history by Markov [7]), and continues to be an active area of research [8]. The purpose of this section is not to review the upscaling of diffusion, but to provide a short example as to how the geometric theorems arise in applications.

2.1. Microscale balance equations

We have adopted the process of pure diffusion in a porous medium because it is one of the simplest transport process that can be analyzed, and because it is a classical problem that is familiar to many. The problem of diffusive transport arises, for example, in a catalytic pellet [9]. We have illustrated a multiscale catalytic reactor in Fig. 1. Here, three physical length scales are apparent: the size of the reactor (length), the size of a typical catalyst pellet (L), and the typical size characterizing the internal microporous structure of the catalyst itself (ℓ_{γ}). We are focused on upscaling the process of diffusion that occurs in the pores of the catalytic pellet (with length scale ℓ_{γ}) up to a new resolution by averaging over the domain $\mathscr{V}$ (with characteristic length scale, r_0). The practical advantage for doing this is that, assuming that the microporous structure of the pellet is reasonably similar from place to place within the pellet, we can then treat the pellet as a single continuum resolved at a scale of, r_0, rather than having to resolve the process at the substantially smaller scale, ℓ_{γ}.

To start, we begin by defining the domain of a single pellet as containing a fluid phase, a solid phase, and an interface; here we denote the fluid as the γ-phase the solid as the κ-phase (Fig. 1). The process of diffusion of a dilute chemical species within the microporous catalytic pellet can be given by (assuming that continuum conditions hold, e.g., [9])

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